Yield spectra and the continuous-slowing-down approximation[†]

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Received 6 May 1977

Abstract. The continuous-slowing-down approximation (CSDA) and the modified discreteenergy-bin (MDEB) method are used to calculate a yield spectra $U(E,E_0)$ in $(eVs)^{-1}$ of electrons with energy E resulting from a primary of energy E_0 . The results of the two calculations are then compared. The MDEB method is found to produce consistently more ions per energy loss while at the same time producing less excitations of some of the low-lying states when compared with the CSDA. These discrepancies can be explained by studying the contributions from the individual generations of electrons to the yield spectra. We also present here an integral equation for the solution of the yield spectra. With this equation, we show that the yield spectra can essentially be calculated if we have knowledge of the primary yield spectrum and $p_1(E,T)$ (in eV^{-1}), the probability for production of a secondary with energy T resulting from a primary of energy E.

1. Introduction

The continuous-slowing-down approximation (CSDA) first developed by Bohr (1913, 1915) for fast heavy particles continues to serve a major role in descriptions of charged-particle degradation. Green and Barth (1965) adapted the CSDA for moderate-energy electrons (below 30 keV) by basing the method upon detailed atomic cross sections (DACS). Using these DACS, Peterson (1969) developed a discrete-energy-bin (DEB) method of energy deposition which allows for the discrete nature of electron energy losses. This work pointed to certain differences between the CSDA and DEB calculation results for He and N_2 , in particular that even at the higher energies (greater than 200 eV), the DEB method tends to predict higher populations of some excited states than does the CSDA.

Garvey and Green (1976), in a more general examination of differences of various energy-apportionment methods, found that the DEB method used with the same DACS leads to the same energy apportionment as the Fowler (1922)‡ equation (and hence, the Spencer–Fano equation (Spencer and Fano 1954)) and the Monte-Carlo collisional simulation approach (Berger 1963).

Green et al (1977, to be referred to as GGJ) have recently formulated another DACs energy-apportionment method which embodies the work of Peterson (1969), Jura (1971), Dalgarno and Lejeune (1971), Cravens et al (1975), Garvey et al (1977)

[†]Supported in part by NASA Grant No NGL-10-005-008.

[‡] See also: Miller W 1957 PhD Thesis Purdue University.

and Green et al (1977). This method, which will be referred to as the modified discrete-energy-bin method (MDEB), leads to a so-called 'yield spectra' $U(E, E_0)$, a powerful function of two variables which is closely related to the Spencer-Fano (1954) degradation spectra (DS) or the equilibrium flux (EF) of Jura (1971). The yield spectra behaves in a much simpler manner than the DS or EF and hence is more amenable to physical interpretation, analytic representation and convenient application.

This $U(E, E_0)$ is the equilibrium number of electrons per unit energy at an energy E resulting from the energy degradation of an incident electron of energy E_0 . It can be used to calculate the total population $J_j(E_0)$ of any state j produced in the course of such a degradation by means of

$$J_{j}(E_{0}) = \int_{E_{j}}^{E_{0}} p_{j}(E') U(E', E_{0}) dE'$$
(1)

where $p_j(E')$ is the probability that an electron with energy E' would excite the jth state of the medium through which it is passing.

Recently Jackman et al (1977, to be referred to as JGG) updated the DACS for Ar, H₂, H₂O, O₂, N₂, O, CO, CO₂ and He. Using these updated cross sections Green et al (1977, to be referred to as GJG) have calculated the yield spectra for these gases and obtained analytic representations for them. This work also examines differences between ion yields calculated by numerical yield spectra, analytic yield spectra and the CSDA method. The pattern of these results suggested that earlier work had not yet completely characterised the differences between the discrete-energy-loss methods and the continuous-slowing-down approximation. The present work is an attempt to do so. Towards this end we first develop a general integral equation for yield spectra. Then by breaking the CSDA and MDEB yield spectra into contributions from various generations of electrons, we seek to arrive at some fundamental physical insight into the differences between results obtained from the CSDA and discrete-energy-loss methods.

In making comparisons we use the two gases O_2 and He. O_2 was chosen because, unlike N_2 in Peterson's (1969) study, it has low-lying forbidden states (namely, b $^1\Sigma_g^+$, a $^1\Delta_g$ and A $^3\Sigma_u^+$ with thresholds of 1.64, 0.98 and 4.50 eV, respectively). It had been noticed by GJG that the populations of these states are higher in the CSDA than they are in the DEB method for incident energies of 10 keV or less. For the other states in O_2 , except the lowest allowed state (B $^3\Sigma_u^-$ with a threshold of 8.4 eV), the DEB approach predicted higher populations than did the CSDA for incident energies above 200 eV.

To provide a simple atomic example we have formulated a simplified three-state mock-up of the He atom (denoted by \widetilde{He}) to test our degradation calculations. Our \widetilde{He} cross section includes only the 2^1P , 2^3S and the ionisation state \widetilde{He}^+ . The forms of these cross sections and their parametric values are given in table 9 in JGG. The O_2 cross sections are the same as those presented in table 4 of JGG.

2. Yield spectra from the DEB and CSDA methods

Because of the linear nature of the degradation process, which is reflected in the linearity of the Spencer-Fano equation (Spencer and Fano 1954, Douthat 1975) for

the degradation spectrum $U(E, E_0)/\sigma_T(E)$ where $\sigma_T(E)$ is the total inelastic electron impact cross section, we can write

$$U(E, E_0) = U_0(E, E_0) + U_1(E, E_0) + U_2(E, E_0) + \dots$$
 (2)

Here $U_i(E,E_0)$ is the contribution to the yield spectrum due directly to the *i*th generation of secondary electrons and $U_0(E,E_0)$ is the contribution due solely to the degradation of the primary electron excluding all secondary electrons. We can use this linear property to obtain a different integral equation for the yield spectrum which will illuminate some of the properties of the yield spectrum and which will facilitate a comparison between the discrete and the CSDA approaches to energy apportionment. We will use the following definitions: $\sigma_j(E)$ is the electron impact cross section for the excitation of the state j by an electron of energy E; $S_i(E,T)$ is the differential cross section for the production of a secondary electron of energy T arising from the excitation of the Tth ionisation continuum of the medium with ionisation potential T0 by an electron of energy T1 and T2 we also define the probability T3 as the probability for the excitation of the state T4 by an electron of energy T5 and T5 and T6 as the probability for the excitation of the state T6 by an electron of energy T7 and T8 as the probability per unit energy that an electron of energy T3 will cause an ionisation resulting in the production of a secondary with energy T5.

Several years ago, Peterson and Green (1968, to be referred to as PG) developed an integral equation for the total population J_j , of the jth state of a medium due to the complete degradation of an incident electron. If we write this equation as an equilibrium production of the populations per unit time, we find that the $J_j(E_0)$ is directly proportional to K, the number of primaries of energy E_0 entering the medium per unit time (which we assume to be one electron per second), and is given by

$$J_{j}(E_{0}) = J_{j}^{0}(E_{0}) + \int_{E_{j}}^{E_{0}} dT \, n(E_{0}, T) J_{j}(T).$$
(3)

Here $J_j^0(E_0)$ is the contribution to the population due directly to the primary electron and $n(E_0, T)dT$ is the total number of secondary electrons with energy between T and T+dT produced directly by the primary in the course of its degradation. In the past, equation (3) has been used primarily in the context of the CSDA; however, the equation itself gives an accurate generation-by-generation accounting of the contributions to the total population of any excited state provided the correct values of $J_i^0(E_0)$ and $n(E_0, T)$ are used (Garvey and Green 1976).

The equilibrium population $J_j(E_0)$ can also be obtained from the yield spectra by using equation (1) or the corresponding equation in terms of the Spencer-Fano (1954) degradation spectra (Inokuti *et al* 1975). Using equations (1) and (2) we see that an exact expression for $J_j^0(E_0)$ is

$$J_j^0(E_0) = \int_{E_j}^{E_0} dE \, p_j(E) \, U_0(E, E_0) \tag{4}$$

with U_0 obtained directly from a modification of the DEB approach (GJG, Garvey et al 1977). Substituting equations (1) and (4) into equation (3), we can obtain

$$\int_{E_j}^{E_0} dE \, p_j(E) U(E, E_0) = \int_{E_j}^{E_0} dE \, p_j(E) U_0(E, E_0) + \int_{E_j}^{E_0} dT \int_{E_j}^{T} dE \, n(E_0, T) p_j(E) U(E, T). \tag{5}$$

Changing the order of integration in the second term on the right-hand side of equation (5) and making the proper change of integration limits, we can write

$$\int_{E_{j}}^{E_{0}} dE \, p_{j}(E) \, \left(U(E, E_{0}) - U_{0}(E, E_{0}) - \int_{E}^{E_{0}} dT \, n(E_{0}, T) U(E, T) \right) = 0. \tag{6}$$

In order for equation (6) to be true for any state and for any incident energy, the quantity inside the large parentheses must be zero or

$$U(E, E_0) = U_0(E, E_0) + \int_E^{E_0} dT \, n(E_0, T) U(E, T). \tag{7}$$

The quantity $n(E_0, T)$ is simply the integral of the product of the probability $p_1(E, T)$ and the number of electrons of energy E due solely and directly to the degradation of an electron starting with an energy E_0 or

$$n(E_0, T) = \int_{2T+I}^{E_0} dE \, p_{\rm I}(E, T) U_0(E, E_0) \tag{8}$$

where I is the minimum ionisation potential of the medium. The lower limit of integration in equation (8) arises from the fact that the secondary electron is defined as the less energetic of the two electrons leaving an ionising event. According to this definition, $n(E_0, T)$ is defined to be zero for $T > (E_0 - I)/2$ which means the upper limit of the integral over T in equation (7) can be reduced to $(E_0 - I)/2$. Making this change and using equation (8) to substitute for $n(E_0, T)$ we obtain the equation

$$U(E, E_0) = U_0(E, E_0) + \int_E^{(E_0 - I)/2} dT U(E, T) \int_{2T + I}^{E_0} dE' \, p_{\rm I}(E', T) U_0(E', E_0). \tag{9}$$

From equation (9) we see that in order to determine $U(E, E_0)$, one could calculate only $U_0(E, E_0)$ for all incident energies less than or equal to E_0 and all corresponding values of E. Successive terms on the right-hand side of equation (9) arising from successive iterations of equation (9) yield U_1 , U_2 , etc.

We can also use equation (9) to determine the CSDA expressions for the yield spectra $U^{c}(E, E_0)$. The CSDA expression for $J_i^0(E_0)$ is (from PG)

$$J_{j}^{0}(E_{0}) = \int_{E_{j}}^{E_{0}} dE \frac{\sigma_{j}(E)K}{L(E)} = \int_{E_{j}}^{E_{0}} dE \, p_{j}(E) \frac{\sigma_{T}(E)K}{L(E)}$$
(10)

where L(E) is the loss function or stopping power of the medium and is given by (adapted from Green and Barth (1965))

$$L(E) = \sum_{k} \sigma_{k}(E)E_{k} + \sum_{i} \int_{0}^{(E_{0} - I_{i})/2} S_{i}(E, T)(I_{i} + T) dT.$$
 (11)

Comparing equations (10) and (4) and following the same line of reasoning as was used to obtain equation (9), we find

$$U_0^{c}(E, E_0) = \sigma_{T}(E)K/L(E)$$
(12)

where $U_0^c(E, E_0)$ is the CSDA expression for $U_0(E, E_0)$. Thus, in the CSDA, U_0^c is independent of E_0 . Green *et al* (1977) found that the actual U_0 is in fact independent of

 E_0 for $E < 2E_0/3$. Substituting equation (12) into equation (9) we can obtain an integral expression for $U^c(E, E_0)$

$$U^{c}(E, E_{0}) = \frac{\sigma_{T}(E)K}{L(E)} + \int_{E}^{(E_{0} - I)/2} dT U^{c}(E, T) n^{c}(E_{0}, T)$$
(13)

where

$$n^{c}(E_{0}, T) = \int_{2T+I}^{E_{0}} dE \, p_{I}(E, T) \, \frac{\sigma_{T}(E)}{L(E)}$$
(14)

and is the CSDA expression for $n(E_0, T)$ (Peterson and Green 1968). Successive iterations of equation (13) yield expressions for U_1^c , U_2^c ,... of the form

$$U_1^{c}(E, E_0) = \frac{\sigma_{T}(E)K}{L(E)} \int_{E}^{(E_0 - I)/2} dT \, n^{c}(E_0, T)$$
 (15)

and

$$U_2^{c}(E, E_0) = \frac{\sigma_T(E)K}{L(E)} \int_E^{(E_0 - I)/2} dT \, n^{c}(E_0, T) \int_E^{(T - I)/2} dT' \, n^{c}(T, T'). \tag{16}$$

Alternatively, again changing the order of integration and making the appropriate changes in the limits of integration, we can write

$$U_2^{c}(E, E_0) = \frac{\sigma_T(E)K}{L(E)} \int_E^{(E_0 - 3I)/4} dT \, n_3^{c}(E_0, T)$$
 (17)

where the tertiary spectrum $n_3^c(E_0, T)$ is given by

$$n_3^{\rm c}(E_0, T) = \int_{2T+I}^{(E_0-I)/2} n^{\rm c}(E_0, E) n^{\rm c}(E, T) \, \mathrm{d}E.$$
 (18)

For practical calculations, except for deposition involving incident energies well above 10 keV, the major contributions to the yield spectra and to the populations of any state come from the primary and the first generation of secondaries; the contributions from higher generations are negligible. We refer the reader to discussions of this point in Khare (1970), Rees et al (1969) and GGJ.

Fano and Spencer (1975), using a quasi-scaled-degradation spectrum approach, have developed an elaborate scheme for deriving a scaled-degradation spectrum on a generation-by-generation basis. Their approach apparently yields an integral equation for the primary contribution to this scaled-degradation spectrum and a coupled set of integral equations for the contributions from higher generations of electrons. Our equation (9) has more direct physical information and involves no scaled quantities. Successive iterations of equation (9) show that the exact contribution to the yield spectrum from any generation of electrons is simply the product of the primary yield spectrum and the initial undegraded distribution of that generation of electrons (see equations (15)–(17)).

With equations (12), (15) and (17) we are thus able to find the CSDA expressions for the yield spectra for the first three generations (other generations can be found quite easily using an extension of the procedure we described above in finding $U_1^c(E, E_0)$ and $U_2^c(E, E_0)$). We see from these equations that the secondary and tertiary

yield spectra depend on the primary yield spectrum and the secondary electron distribution. In the next section we will apply these equations to \widetilde{He} and O_2 .

It was shown in GJG that the yield spectrum from the MDEB method could be modelled accurately using the analytical expression

$$U(E, E_0) = \{ A[(\xi_0^{1-t}/\epsilon^{\frac{3}{2}+r}) + b\xi_0^s] \theta(E_0 - E - E_\theta) + \delta(E_0 - E) \} K.$$
 (19)

Here, θ is the Heaviside function with E_{θ} , the minimum threshold of the states considered, $\delta(E_0-E)$ is the Dirac delta function, K has been defined previously, $\xi_0=E_0$ (in eV)/1000 and $\epsilon=E/I$. A and b are the principal parameters and r, s and t are small parameters.

In equation (19) we note that the last term is considered to be the source term. We will assume K to be 1 electron per second. For the purposes of discussion and illumination of the differences between the CSDA and the MDEB methods that will be pointed out later in this paper, we can make the following assumption about the source term from the MDEB approach. This source term could be assumed to be a flux centred at $500 \, \text{eV}$ over a $1 \, \text{eV}$ bin width from $499.5 \, \text{eV}$ to $500.5 \, \text{eV}$ of $1 \, \text{electron/(eV s)}$ in the system.

3. Discussion

We used equations (12), (15) and (17) with a numerical integration (using the trapezoidal method because of the relatively smooth functions) to find the yield spectra from the CSDA for a primary of energy 500 eV for O_2 and \widetilde{He} and compared these yield spectra contributions with the MDEB yield spectra. The results are shown in figure 1 for \widetilde{He} . Here, for the primary yield spectrum, the $U_0^c(E, E_0)$ values are larger

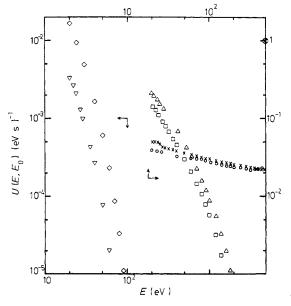


Figure 1. Primary, secondary and tertiary yield spectra from \widetilde{He} from the CSDA and MDEB methods for a primary energy E_0 of 500 eV as functions of energy E. Note the changes of axes for the right-hand side of the figure. The points are as follows: \times primary yield CSDA; \square secondary yield CSDA; \triangledown tertiary yield CSDA; \bigcirc primary yield MDEB; \triangle secondary yield MDEB; \diamondsuit tertiary yield MDEB; \bigotimes source term.

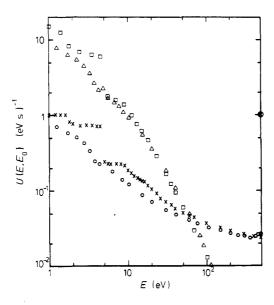


Figure 2. Primary and secondary yield spectra from O_2 from the CSDA and MDEB methods for a primary energy E_0 of 500 eV as functions of energy E. The points are as follows: \times primary yield CSDA; \square secondary yield CSDA; \bigcirc primary yield MDEB; \triangle secondary yield MDEB; \bigotimes source term.

than the correct $U_0(E,E_0)$ (from the MDEB method) out to about $420\,\mathrm{eV}$, but $U_1^c(E,E_0)$ and $U_2^c(E,E_0)$ are consistently smaller than $U_1(E,E_0)$ and $U_2(E,E_0)$, respectively. Subsequently, the dominance of the $U_1(E,E_0)$ is seen and the populations resulting from all three states in our He mock-up should be greater with the DEB method. This is seen in the complete calculation.

With O_2 (see figure 2) we only present the primary and secondary yield spectra as the tertiary yield spectrum is miniscule by comparison. We note a similar type of behaviour for the $U_0(E, E_0)$ to that which was seen with \widetilde{He} . We again find that the $U_0^*(E, E_0)$ values are larger out to about 420 eV. The secondary yield spectra behaviour is more curious in O_2 . Out to roughly 25 eV the $U_1^*(E, E_0)$ is higher, but there is a crossing of the curves near this energy and the $U_1(E, E_0)$ is larger from this point on. The main contribution for the low-lying forbidden states, which were found to have higher populations with the use of the CSDA, is from energies between 1 and 20 eV where both the $U_0^*(E, E_0)$ and $U_1^*(E, E_0)$ are larger than their MDEB counterparts. The low-lying allowed state which also has a larger population from CSDA seems to be right on the borderline for the over-contribution below 25 eV from $U^*(E, E_0)$ and the under-contribution above 25 eV from $U^*(E, E_0)$. Its population

Table 1. Here we present a model gas with a comparison between the CSDA and the MDEB primary yield spectra. $U_0^c(E, E_0)$ and $U_0(E, E_0)$ are given at 10 eV intervals for the degradation of a primary of energy 100 eV.

Energy (eV)	100	90	80	70	60	50	40	30	20	10
$U_0(E, E_0)$ $U_0^{\circ}(E, E_0)$	0·100	0·050	0·058	0·062	0·059	0·060	0·060	0·060	0·060	0·066
	0·060	0·060	0·060	0·060	0·060	0·060	0·060	0·060	0·071	0·100

is, in fact, close to the same from either the CSDA or the MDEB methods. The other high-lying states show the dominance of the higher energy $U_1(E,E_0)$ and $U_0(E,E_0)$ values so that the populations from these other states are always predicted to be higher from the MDEB method.

Since both of these gases showed the same behaviour in the comparison of $U_0^c(E, E_0)$ and $U_0(E, E_0)$, it is appropriate to attempt to find the reason behind this conduct. We will use a hand calculation in this endeavour. In this hand calculation, we assume a gas with three allowed states of thresholds 10, 20 and 30 eV. Assume the probabilities for exciting these states goes respectively as $\frac{1}{2}$, $\frac{1}{3}$ and $\frac{1}{6}$, and are constant throughout the energy regime. We will degrade a 100 eV primary in both the MDEB and CSDA methods. Using 10 eV bin widths we are able to calculate a $U_0(E, E_0)$ and $U_0^c(E, E_0)$ given in table 1. The $U_0(E, E_0)$ is found using the approach described in GGJ. We can rewrite the expression in equation (12) for $U_0^c(E, E_0)$ as

$$U_0^{c}(E, E_0) = \left(\sum_{j=1}^{3} W_j p_j\right)^{-1}$$
 (12')

where W_j is the threshold for the jth state and p_j is the probability for exciting the jth state.

We realise that the thresholds we took for our states as well as the energy-bin widths are such that they allow for the best comparison between the CSDA and the MDEB methods. If we had taken 5 eV bin widths, for example, the MDEB would have predicted 0·0 yield spectra in every other bin and twice as much of a yield in the interposing bins. The average yield spectra, however, from $U_0(E,E_0)$ would have been the same as that presented in table 1.

The same type of behaviour is noted for this gas that was observed for \widetilde{He} and O_2 . At the low energies (say 20 and 10 eV) the $U_0^c(E, E_0)$ is above the $U_0(E, E_0)$ but at the high energy of 100 eV the $U_0(E, E_0)$ is above. In the intermediate region, the $U_0(E, E_0)$ and $U_0^c(E, E_0)$ are very similar.

We have shown in equations (15) and (17) that the secondary and tertiary yield spectra depend directly on the primary yield spectrum. Thus we feel that explaining the differences between the primary yield spectra from the CSDA and MDEB methods will go a long way towards explaining the differences found in the populations calculated in both methods of energy degradation. We will, therefore, elucidate these differences.

The CSDA approach does not take into account what happened to the primary electron before it enters a certain energy regime, i.e. $U_0^c(E, E_0)$ depends only on E and not on E_0 (see equation (12)). The degraded primary is 'blind' to its previous history. At the primary energy E_0 there is no source term for the electron, but the $U_0^c(E, E_0)$ derived at that energy, say $500\,\mathrm{eV}$, is the same as for an electron with any larger E_0 . The absence of this source term and the ramification of this absence have apparently been overlooked by other investigators. At the low energies, any state's contribution to $U_0^c(E, E_0)$ cuts off once E is below the threshold of that state. This causes the CSDA to predict non-physical structure in the low-energy region of the yield spectra and causes the $U_0^c(E, E_0)$ to be larger because essentially the average energy loss $\langle W \rangle$ for an excitation is too small. Here we see $\langle W \rangle = L(E)/\sigma_T(E)$ (see figure 2).

The $U_0(E, E_0)$ from the MDEB method is affected very much by the previous history of the electron. There is a source term at the incident energy which allows for the

contribution to the $U_0(E,E_0)$ from the electron at the incident energy. The Heaviside function in equation (19) allows for the zero contribution to $U_0(E,E_0)$ for energies between E_0 and E_0-E_θ . At the low energies there are contributions to $U_0(E,E_0)$ in energy intervals centred on E from states with thresholds greater than E, so that the average energy loss at the lower energies is greater from the MDEB method. This would tend to decrease the $U_0(E,E_0)$ at these low energies.

From the preceding discussion of the primary yield spectra, we can understand the differences resulting in the other generation contributions. In the CSDA, $U_1^c(E, E_0)$ (from equation (15)) depends on $U_0^c(E, E_0)$ and $n^c(E_0, T)$. The $n^c(E_0, T)$, also, depends on the $U_0^c(E', E_0)$ values from E' = 2T + I up to E_0 given in equation (14). Paralleling the CSDA course, we have that

$$U_1(E, E_0) = \int_E^{(E_0 - I)/2} dT \, n(E_0, T) \, U_0(E, T)$$
 (20)

and that $n(E_0, T)$ is related to the $U_0(E, E_0)$ by equation (8).

We see in both He and O_2 that above about $T = E = 25 \,\mathrm{eV}$ the $U_1^c(E, E_0)$ is lower than the $U_1(E, E_0)$. For an ionisation threshold of $I = 15 \,\mathrm{eV}$ we get $2T + I = 65 \,\mathrm{eV}$. In equations (8) and (14) we find the $n(E_0, T)$ and $n^c(E_0, T)$, respectively. The source term in $U_0(E, E_0)$ dominates the difference between the two secondary electron distributions. The $U_0^c(E, E_0)$ and $U_0(E, E_0)$ values are close to the same above $E = 65 \,\mathrm{eV}$ and amount to at most $0.05/(\mathrm{eV}\,\mathrm{s})$. Thus the domination of the source of 1 electron/(eV s) can be easily seen.

Below $T = E = 25 \,\mathrm{eV}$ the $U_1^c(E, E_0)$ may be lower or higher than the $U_1(E, E_0)$. In the case of $\widetilde{H}e$ there is a cut-off at the lowest threshold of about 20 eV, but in O_2 we are given a lowest threshold of 1 eV and are able to observe more carefully the differences in the secondary yield spectra. At these lower energies the $U_0^c(E, E_0)$ has comparable values with the source term from $U_0(E, E_0)$ and thus it is not clear which secondary yield spectra should be greater. In the case of O_2 , the $U_1^c(E, E_0)$ dominates the $U_1^c(E, E_0)$.

If one were to 'doctor-up' the CSDA approach by adding a source term at the incident energy, this would over-correct the $U_0^{\rm c}(E,E_0)$ values. We tried such a correction for O_2 and it resulted in an over-population of all states at any energy. At the higher energies (above 200 eV), the higher-lying state populations from the CSDA method turned out to be very close to the populations from the MDEB approach, but at the lower energies (200 eV and below) the result was a very high over-population of all states by the CSDA method.

In GJG, we noted that the eV per ion pair was always lower for the MDEB method of energy deposition with all nine gases studied in that paper. This suggests then that our discussion of the comparison between the CSDA and the MDEB approaches can be used for any gas. The lowest-lying forbidden states (with thresholds below about 8 eV) and vibrational levels will tend to have their populations overestimated by the CSDA method because most of their population results from the energies of $E \simeq 30 \, \text{eV}$ and below where the $U^c(E, E_0)$ tends to be larger than the $U(E, E_0)$. The higher-lying states (with thresholds above 8 eV) will tend to have their populations underestimated by the CSDA method. Above $E \simeq 30 \, \text{eV}$, the $U^c(E, E_0)$ tends to be smaller than the $U(E, E_0)$ where the source term of the $U(E, E_0)$ is included. This is the region of the most contribution to these higher threshold states.

4. Conclusions

In this paper we have pointed out the differences between two methods of solution of the energy degradation problem. The CSDA is the more naive method of energy degradation and fails to model correctly an electron's energy deposition. This is mainly due to the shortcoming of the CSDA in not utilising the history of the electron's degradation. The MDEB, on the other hand, distributes the energy more correctly into the various states. This method not only allows for the electron's previous history in the degradation, but also takes the discrete nature of the energy-loss process into account.

In addition, we have presented an integral equation for the yield spectra by which $U(E,E_0)$ can be determined from $U_0(E,E_0)$. The calculation of $U_0(E,E_0)$ is straightforward in the MDEB approach and, as was found in GGJ, $U_0(E,E_0)$ is a very smooth and regular function for $E < E_0 \simeq 100 \, \mathrm{eV}$, i.e. outside of the energy region dominated by the rapid fluctuations produced by the discrete nature of the deposition process. In fact, for values of E_0 above several hundred eV, $U_0(E,E_0)$ is independent of E_0 for $E < 2E_0/3$.

Acknowledgments

The authors would like to thank Dr G J Kutcher for helpful discussions concerning the changing of integration orders in equation (5) and Dr R A Hedinger for several helpful discussions on the nature of the deposition process.

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